

Kinetic roughening and phase ordering in the two-component growth model

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Abstract

Interplay between kinetic roughening and phase ordering is studied in a growth SOS model with two kinds of particles and Ising-like interaction by Monte Carlo simulations. We found that, for a sufficiently large coupling, growth is strongly affected by interaction between species. Surface roughness increases rapidly with coupling. Scaling exponents for kinetic roughening are enhanced with respect to homogeneous situation. Phase ordering which leads to the lamellar structure persisting for a long time is observed. Surface profiles in strong coupling regime have a saw-tooth form, with the correlation between the positions of local minima and the domain boundaries.

Key words: Computer simulations; Ising models; Growth; Surface roughening; Surface structure, morphology, roughness and topography.

PACS: 81.10.Aj, 68.35.Ct, 75.70Kw

1 Introduction

Growth by vapour deposition is a technologically important process for producing high quality materials. During last years much progress has been made in understanding of growth mechanisms on the microscopic level [1]. However, these results refer mainly to single-component homogeneous growth and

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growth of binary materials is much less understood. Essential feature in binary systems is phase ordering [2]. Recently there was interest in interplay between phase ordering during growth and kinetic roughening [3–5]. Kinetic roughening is one of the important aspects of crystal growth. Due to stochastic fluctuations during a deposition process the growing surface becomes rough and roughness typically increases with time as a power with a characteristic exponent β . This is important from the practical point of view, besides kinetic roughening also attracted a lot of interest in the context of non-equilibrium statistical mechanics [6].

In this paper we discuss the interplay between compositional ordering and kinetic roughening in a simple model for growth of binary alloys which we recently formulated [5].

2 Model

Our model is based on the single-step solid-on-solid geometry. We confine ourselves here to one-dimensional substrate with the coordinate i . The surface is described by a single-valued function $h_i(t)$ with the additional constraint $|h_i - h_j| = 1$ for neighbouring sites i and j . A new particle can be added only at a growth site corresponding to a local minimum in the surface height profile. We consider two types of particles, which we distinguish by a variable σ taking the value $+1$ or -1 . Growth rules are controlled by a change of energy of alloy after deposition of a new particle. The energy is given by the Ising-like interaction. The probability of deposition of a new particle of type σ to a growth site i is proportional to $\exp(-\Delta E(i, \sigma)/k_B T)$; k_B is Boltzmann's constant and T is temperature. The change of energy is $\Delta E(i, \sigma)/k_B T = -K\sigma [\sigma(i-1) + \sigma(i) + \sigma(i+1)] - H\sigma$. Here K is a dimensionless coupling strength and H is an external field. We call this model a two-component single-step (TCSS) model. We consider here only the case of zero external field.

The surface roughness is described by the surface width $w(t, L) = \langle \sqrt{h^2 - \bar{h}^2} \rangle$, where t is the time, L is the linear size and the bar denotes a spatial average, $\langle \dots \rangle$ a statistical average. Ordering is studied by the time evolution of the average domain size along the surface $D(t)$.

3 Results

We performed extensive simulations for various values of K . Evolution of the surface profile is affected by composition of the surface, in particular it de-

depends on composition of the initial flat substrate. We considered three different types: i) a neutral substrate, i.e. without any interaction with deposited particles, ii) an alternating substrate, with alternating types of particles and iii) a homogeneous substrate composed of one type of particles.

Evolution on the neutral and the alternating substrate is almost the same. In Fig. 1 we can see that the effective exponent ($\beta_{\text{eff}} = 0.45$) is at first larger than the exponent for homogeneous growth, $\beta = 1/3$, which corresponds to the so-called Kardar-Parisi-Zhang (KPZ) class [7]. However, after a certain time $t_{\text{cross}} \approx 10^3$ the effective exponent crosses over to the value close to $1/3$ ($\beta_{\text{eff}} = 0.32$). This behaviour can be explained by evolution of compositional ordering. In the inset of Fig. 1 we present time dependence of the average domain size for three substrate types considered. We can see that for all of them the domain size saturates at time close to t_{cross} . Hence, ordering of the surface leads to enhanced increase of the roughness, but when ordering stops the surface roughness increases further with the same exponent as in one-component single-step growth model.

In the case of the homogeneous substrate the behaviour of the surface width changes dramatically (cf. Fig. 1). The general features are the following. At first the width starts to grow with the exponent close to $1/3$ (this regime is extended over several decades of deposition time for very strong coupling). It is caused by the fact that practically no domains with minority type of particles are formed because probability to nucleate these domains is rather small; growth is the same as in the pure single-step model. Then the slope crosses over to a very large value ($\beta_{\text{eff}} = 1.15$). This unexpected effect is related to growth of trapezoidal features with the length given by positions of the minority type domains, which start to appear but often again quickly disappear. The rapid

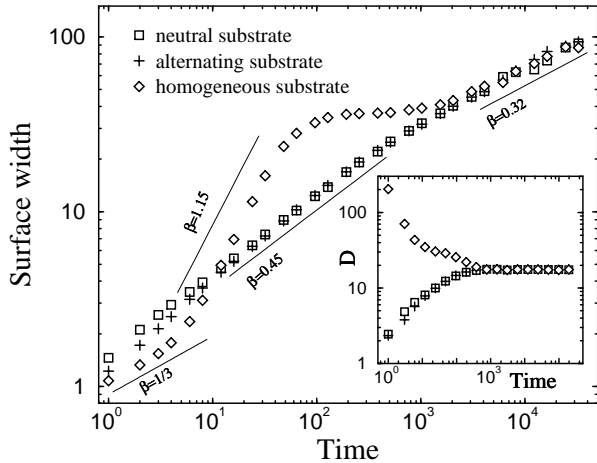


Fig. 1. Surface width w vs. time for coupling strength $K = 1.0$, and three different types of the substrate of size $L = 10000$. Data are averaged over 30 independent runs. The values of slope, $\beta = 0.45$ and $\beta = 0.32$, were obtained by fit to points for the alternating substrate, the straight line with slope $1/3$ is only guide for eye.

increase of roughness ceases when relatively stable minority type domains are nucleated. The further increase of roughness is very slow up to the time when the average domain size saturates and growth continues with the KPZ exponent $\beta = 1/3$. We illustrate the difference in evolution on the neutral and on the homogeneous substrate in Fig. 2. We can see that for the homogeneous substrate dark domains appear very slowly.

Let us now turn to the dependence on the coupling K in the case of the neutral substrate. For small K , there is no ordering in the growth direction. Small domains appear and shrink again, but for a larger K the clear lamellar structure exists. We illustrate this in Fig. 3 which shows evolution of configurations on a substrate with periodic domains imitating the lateral superlattice. We can see that for $K = 2$ lamellae persist for long time. Notice the correlations between the positions of local minima of surface profile and domain boundaries. We observed that this is a typical case for stronger coupling independently

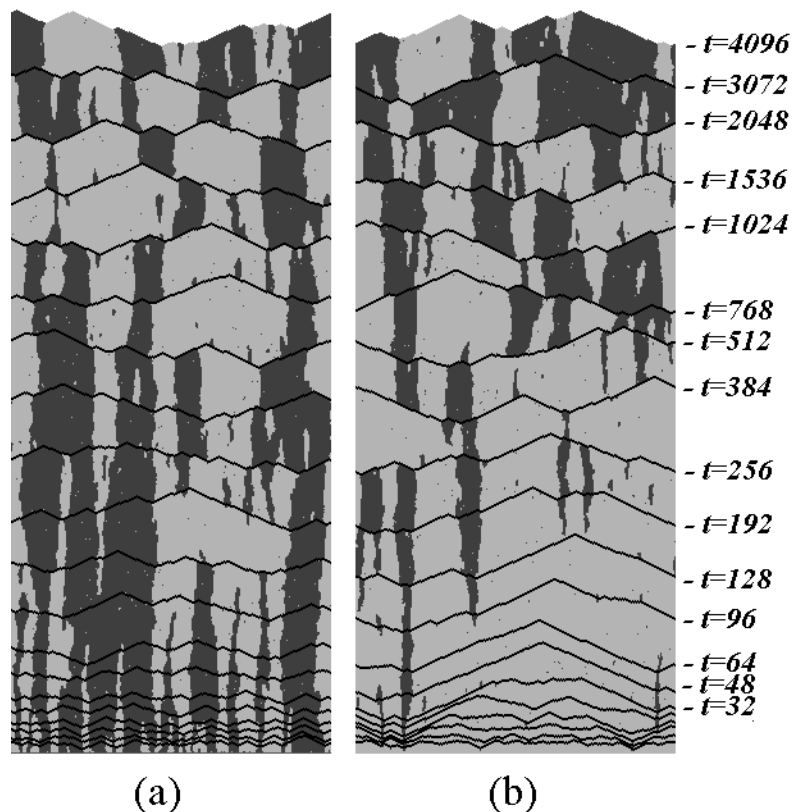


Fig. 2. Examples of evolution of surface profiles for $K = 1.0$, and two different substrates: (a) the neutral substrate and (b) the homogeneous substrate. Surface profiles at various times increasing as powers are indicated by black lines, only part of the grown material close to the surface is shown for given time. Dark and light grey correspond to different types of particles. System size is $L = 250$.

on the type of the substrate. We have found that the roughness increases

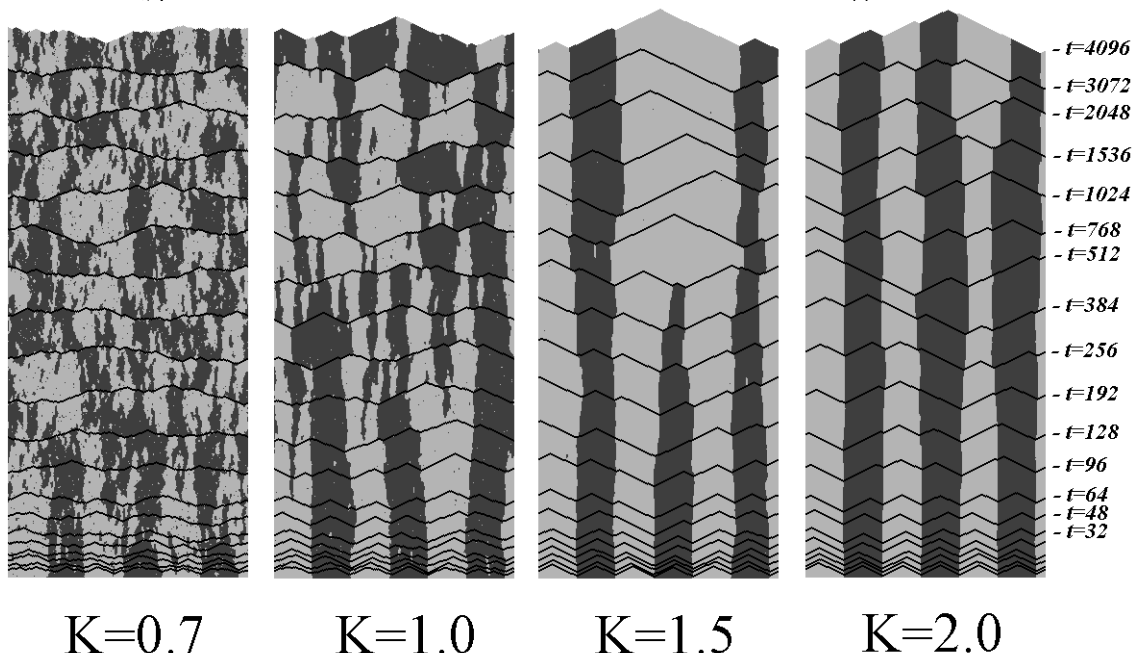


Fig. 3. Examples of evolution of surface profiles on the substrate with alternating domains of different particle types for several coupling strengths K . Meaning of colours and other conditions are the same as in Fig. 2.

rapidly with the coupling. The effective exponent β_{eff} for initial growth increases with K and it seems to approach the value $1/2$; for $K = 2$ we have found $\beta = 0.52 \pm 0.02$. The crossover time for change of β_{eff} to the KPZ exponent is also increasing rapidly with K ($t_{\text{cross}} \propto e^{\gamma K}$ with $\gamma \approx 3.5$).

4 Conclusion

We demonstrated that phase ordering leads to faster kinetic roughening than in the homogeneous case. However, after some time this behaviour crosses over to the ordinary behaviour for homogeneous growth. But the crossover time increases rapidly with interaction between particles, so practically only the regime with enhanced roughness can be seen for stronger coupling. We also illustrated the strong sensitivity of evolution on the initial composition of the substrate.

Acknowledgement

This work was supported by grant No. A 1010513 of the GA AV ĆR.

References

- [1] For review, see: A. C. Levi and M. Kotrla, J. Phys.: Condens. Matt. 9 (1997) 299.
- [2] A. J. Bray, Adv. Phys. 43 (1994) 357.
- [3] J. R. Smith, Jr and A. Zangwill, Phys. Rev. Lett. 76 (1996) 2097.
- [4] F. Léonard, M. Laradji, and R. C. Desai, Phys. Rev. B 55 (1997) 1887.
- [5] M. Kotrla and M. Předota, Europhys. Lett. at press.
- [6] J. Krug, Adv. Phys. 46 (1997) 139.
- [7] M. Kardar, G. Parisi, and Y.C. Zhang, Phys. Rev. Lett. 56 (1986) 889.